QUANTA CHEMISTRY

An Institute of Chemical Sciences

CSIR-NET | IIT-GATE | IIT-JAM | Other MSc. Entrance

DPP- (1) Electron spin Resonance Spectroscopy

1. ESR spectroscopy falls under which of the following region

   (a) Radiofrequency region (b) Microwave region

   (c) UV-visible region (d) Infrared region

2. Which of the following systems can show ESR Spectroscopy?

   (a) The systems which are concerned with splitting of nuclear spin states

   (b) Splitting of electronic spin states is considered

   (c) Free radical intermediates

   (d) Triplet states

   (a) A, D (b) B, C (c) B, C, D (d) A, D

3. What one of the following molecules will show ESR signal?

   (a) N_2 (b) C_2 (c) F_2 (d) O_2

4. What is the source of radiation in ESR?

   (a) Klystrone valve (b) Tungsten lamp (c) Deuterium lamp (d) Radio activity

5. What will be the frequency of radiation for resonance condition for a free electron placed in a magnetic field of strength 0.3T?

   (a) 8.4 GHz (b) 9.5 GHz (c) 10 GHz (d) 11 GHz

6. Calculate the frequency for an unpaired electron in a magnetic field of strength 0.35T (g = 2).

   (a) 8.4 GHz (b) 9.5 GHz (c) 10 GHz (d) 9.8 GHz

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7. The ESR frequency for a free electron in 9000 MHz. Calculate the magnetic field at which ESR spectrometer is working (g = 2) _____. (mT)

8. How many of the following species are ESR active _____ Ni^{2t}, Cu^{2t}, VO^{2t}, $(SO_3)_2$ NO^-, B_2, (O_3, $KMnO_4$, C_2H_5)

9. The ESR spectrum of methyl radical occurs at 330 mT in a spectrometer operating at 9250 MHz. Calculate the g value of the radical.

   (a) 2.002 (b) 2.003 (c) 2 (d) 2.004

10. At what field would the methyl radical come into resonance in a spectrometer operating 9.5 GHz (g = 2.0026)?

    (a) 0.33T (b) 0.54T (c) 0.9T (d) 1T

11. An irradiated sample of MgO has a strong ESR line at 0.163T, when the spectrometer is operating at 9.4 GHz. What is the g-value of the line?

    (a) 2.1 (b) 2.003 (c) 3 (d) 4.13

12. The reference compound used in ESR spectroscopy is
(a) diphenylpicryl hydrazine dehydrate (b) diphenylpicryl hydrazyl radical
(c) diphenylpicryl hydrazine (d) Diphenyl hydrazine

13. Which of the following species is ESR active.
(a) $Ni(CO)_4$ (b) $[CO(NH_3)_6]^{3+}$ (c) $VOSO_4$ (d) $K_2Cr_2O_7$

14. The correct of Bohr magneton is
(a) $8.99 \times 10^{-24}\ Am^2$ (b) $9.27 \times 10^{-24}\ Am^2$
(c) $5.66 \times 10^{-24}\ Am^2$ (d) $9.27 \times 10^{-28}\ Am^2$

15. Under ideal conditions, a commercial X-band spectrometer can detect the spin of 'x' at room temperature. What is the value of X
(a) 10^{85} (b) 10^{12} (c) 10^{50} (d) 10^{5}

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16. Which of the following statements about ESR spectra is/are correct
(a) Sensitivity of ESR is 1000 times less than that of NMR
(b) It's coupling constant is represented by J.
(c) Relaxation time for the electrons is very less
(d) It uses microwave frequency radiation

17. Which of the following statements is/are correct about ESR.
(a) ESR spectra of the odd electron having single mode
(b) ESR spectra are easy to locate in derivative mode
(c) The g value for the single electron is 2.0023
(d) DPPH is used as the reference compound in ESR

18. Which of the following statements is/are correct?
(a) Cr^{3t} and Cu^{+} are ESR active ions.
(b) The frequency associated with electron having spin 'S' in magnetic field Bz is represented as
$\nu = \frac{\mu_B Bz}{h}$ (μ_0-Bohr magneton)
(c) ESR sensitivity increases with decreases in temperature
(d) ESR sensitivity tells us about net absorption of the photons.

19. Which of the following quantities tells about the position of ESR lines?
(a) g-factor (b) coupling constant (c) Bohr magneton (d) Line width

20. What is the exact Experimental value of g?
(a) ±2 (b) 2.002 (c) 2.002 ± 0.003 (d) 2.002 ± 0.01

ANSWER KEY

1.	(b)	2.	(c)	3.	(d)	4.	(a)	5.	(a)	6.	(d)	7.	(321.5mT)
8.	(6)	9.	(a)	10.	(?)	11.	(d)	12.	(b)	13.	(c)	14.	(b)
15.	(b)	16.	(c,d)	17.	(b,c,d)	18.	(c,d)	19.	(a)	20.	(c)		

HINTS & SOLUTION

2.**Sol.** Splitting of nuclear spin states is considered in NMR, not ESR Spectroscopy?

3.**Sol.** O_2 contains unpaired electrons it is paramagnetic in nature.

5.**Sol.** $h\nu = g\beta B_0$

$$\nu = \frac{g\beta B_0}{h} = \frac{2.0023 \times 9.2732 \times 10^{-24}\,JT^{-1} \times 0.3T}{6.626 \times 10^{-34}\,Js}$$

$= 8.4 \times \underline{10}^9$ Hz

$= 8.4$ GHz

10^9Hz = 1 GHz.

6.**Sol.** $$\nu = \frac{2 \times 9.2732 \times 10^{-24}\,JT^{-1} \times 0.35\,JT}{6.626 \times 10^{-34}\,Js}$$

$= 9.8 \times 10^9$ Hz

$= 9.8$ GHz

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7.**Sol.** $B = \frac{h\nu}{g\beta} = \frac{6.626 \times 10^{-34}\ Js \times 9000 \times 10^6 s^{-1}}{2 \times 9.2732 \times 10^{-24}\,JT^{-1}} = 0.3215T = 321.5\ mT$

8.**Sol.** Cu^{2t}, VO^{2t}, $(SO_3)_2$ NO^-, B_2, CO_3, C_2H_5 are ESR active due to presence of unpaired electron in all of them.

9.**Sol.** $g = \frac{h\nu}{\beta B} = \frac{6.626 \times 10^{-34}\,Js \times 9250 \times 10^6 s^{-1}}{9.2432 \times 10^{-24}\,JT^{-1} \times 330 \times 10^{-3}\,T} = 2.002$

10.**Sol.** $\beta = \frac{h\nu}{g\beta} = \frac{6.626 \times 10^{-34}\,Js \times 9.5 \times 10^9\,Hz}{2.0026 \times 9.2732 \times 10^{-24}\,JT^{-1}}$

$= 3.3910^{-1}$ T

$= 0.339$ T

11.**Sol.** $g = \frac{h\nu}{\beta B} = \frac{6.626 \times 10^{-34}\,Js \times 9.4 \times 10^9\ Hz}{9.2732 \times 10^{24}\,JT^{-1} \times 0.163T} = 4.13$

12.**Sol.** 1, 1,-diphenyl-2-picryl hydrazyl free radical (DPPH) is used as reference compound in ESR, due to Extreme stability.

13.**Sol.** Vanadium has oxidation state of +4 (v + 4) and thus $3d^1$, thus it is ESR active.

MSQ

16.**Sol.** (i) Sensitivity of ESR is 1000 times more than NMR.

(ii) There is hyperfine coupling constant which is represented by A.

17.**Sol.** ESR has two modes

- Absorption mode

• Derivative mode

In absorption mode, ESR spectra are broad, thus located in derivative made.

18. Ans.(c, d)

(i) $Cr^{3t} \rightarrow d^3 \rightarrow$ three unpaired electrons $\rightarrow$ ESR active

$Cu^{+} \rightarrow d^{10} \rightarrow$ no unpaired electron $\rightarrow$ ESR inactive

(ii) The frequency is represented as $\nu = \frac{ge\mu_B B_2}{h}$

20. **Sol.** 2.002 is the theoretical value (for free electron) In theoretical calculations, only spin motion is calculated, spin orbital coupling is not taken. But in Experimental value, orbital motion is also considered.